Ab-initio Study on the optical properties and vibrational response of 3C Porous Silicon Carbide

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In the last years there has been an important development on the theoretical and experimental investigations of 3C porous Silicon Carbide (pSiC) due to its potential applications in fast response H sensors, and due to its photoluminescence for uses in optoelectronic appliances. There are plenty of experimental investigations on the synthesis and characterization of pSiC, however there are only a few theoretical studies on this material which could be of great importance to the development of its applications, specially the knowledge of their vibrational and optical properties which would allow for potential applications in thermoelectrics and solar cells. In this work the optical and vibrational properties of pSiC using the first principles Density functional Theory scheme. In first instance the convergence of the optical and vibrational properties of crystalline SiC and a comparison to reported experimental values on the literature was performed, in order to find the best parameters to study the pSiC. The pSiC was modelled by removing atoms in the [001] direction of an otherwise perfect SiC crystal according to the supercell scheme [1,2]. To study the effect of surface passivation on the optical and vibrational properties of pSiC the surface dangling bonds were saturated with H atoms, then pairs of H atoms were replaced with O atoms. Since SiC is a kind of a binary material multiple surface chemistries can be modelled, in this case surface chemistries with only Carbon (C-rich) and Silicon (Si-rich) were selected. Vibrational properties results show that the C-rich surface creates stable structures since there are not negative frequencies in either their phonon density of states or dispersion, whereas the Si-rich case have some negative frequencies in its spectrum which indicates possible mechanical instabilities. The optical activity of the pSiC is enhanced compared to its bulk counterpart which could be important for its application in the electronic industries for optoelectronic devices.